

Transport through a multiply connected interacting meso-system using the Keldysh formalism

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Abstract

We apply the Keldysh formalism in order to derive a current formula easy to use for a system with many sites, one of which is interacting. The main technical challenge is to deal with the lesser Green function. It turns out that, in the case of the left-right symmetry, the knowledge of the lesser Green function is not necessary and an exact current formula can be expressed in terms of retarded Green functions only. The application is done for a triangular interferometer which gives a good account of the Fano-Kondo effect. It is found that the interference effects, in the context of Kondo correlations, give rise to a point in the parameters space where the conductance is temperature-independent. We include a comparison with the results from the Ng's ansatz, which are less accurate, but can be used also in the absence of the above mentioned symmetry.

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I. INTRODUCTION

The transport through mesoscopic systems has been very much discussed in the last years because of promising technological applications, but also for revealing interesting conceptual aspects. The simultaneous consideration of both interaction and interference effects is a nowadays topic in mesoscopic physics and many efforts have been done to overcome the specific theoretical difficulties. One of the main tools is the Keldysh transport formalism, that requires the knowledge of the retarded and lesser Green functions (e.g. [1, 2, 3, 4, 5]). The general expression of the current through the lead indexed by α is :

$$J_\alpha = \frac{2e}{h} \int_{-\infty}^{\infty} d\omega \, i\Gamma_\alpha \{ f_\alpha(\omega) [G_{\alpha\alpha}^r(\omega) - G_{\alpha\alpha}^a(\omega)] + G_{\alpha\alpha}^<(\omega) \} , \quad (1)$$

where f_α is the Fermi distribution function in the α electrode and $\Gamma_\alpha = \pi\tau_\alpha^2\rho$, with the usual notations.

Most of the papers discuss the Single Impurity Anderson Model (SIAM), in which case a simplified version of the formalism can be employed. In this model, the two leads are connected to the same site, which mimics the quantum dot, and in this situation the knowledge of the retarded Green function is sufficient for describing the transport properties (as the lesser Green function is eliminated by current symmetrization)[1]. Only a few papers go beyond this model by introducing in the Hamiltonian a term which produces a short-cut of the impurity, mimicking a mesoscopic ring [6, 7]. In the non-interacting case, eq.(1) can be shown to give the Landauer-Büttiker result, that was widely employed.

The implementation of the Keldysh formalism for the general case of a many-site, multiple connected system with interaction is not trivial. Second order perturbative calculations have been applied for the case of the electron-phonon interaction[3, 4] or in the context of dephasing [5], but such perturbative approaches cannot be applied in the case of strong electronic correlations. Recently, Entin-Wohlman et al. [8] and Kashcheyevs et al. [9] developed an equation-of-motion solution for G^r in any complex geometry described by a tight-binding model, but not for $G^<$. The calculation of $G^<$ in the strong interaction regime is a more difficult task and requires supplementary decoupling approximations [2, 10].

A solution to this problem was also suggested [11, 12] by diagonalizing the interacting Hamiltonian in the slave-boson representation. Then the knowledge of the retarded Green function is sufficient again, but the approach restricts the range of validity of the transport

calculation as the mixed valence regime is not correctly described. Another way to get rid of $G^<$ was proposed in [13] by imposing stationarity conditions on the mean values of some non-hermitic operators, the meaning of which is not obvious to us (especially under non-equilibrium conditions).

In this paper we propose two different approaches. One is to approximate the lesser Green functions by using the Ng's ansatz [14]. Another possibility is to write down the system of equations of motion for $G_{ij}^<$ (where i, j index any site of the system) and express the current (1) in terms of $G_{dd}^<$ and G_{dd}^r (the index 'd' means the interacting site). It will be shown that, for the particular case of left-right and time-reversal symmetry, $G_{dd}^<$ can be eliminated by symmetrization of the current formula. The result is better in this case than by using Ng's ansatz, since no approximations are introduced in the current formula.

The application is done for the triangle system in the inset of Fig.1 which is the simplest multiple connected system with two leads. This system is typical for the study of Fano and Fano-Kondo effects.

II. MODEL AND TECHNIQUES.

Our approach is based on the following Hamiltonian written in a discrete basis :

$$H = \sum_{\mathbf{k}, \sigma, \alpha} (\epsilon_{\mathbf{k}\alpha} - \mu_{\alpha}) c_{\mathbf{k}\alpha, \sigma}^{\dagger} c_{\mathbf{k}\alpha, \sigma} + H_{meso}(\{a_i^{\dagger}, a_i\}) + H_T, \quad (2)$$

where the mesoscopic system contains an interacting site indexed by d :

$$H_{meso} = \sum_{i\sigma} E_i a_{i\sigma}^{\dagger} a_{i\sigma} + \sum_{ij\sigma} (t_{ij} a_{i\sigma}^{\dagger} a_{j\sigma} + H.c.) + H_{int}(a_{d\sigma}^{\dagger}, a_{d\sigma}) \quad (3)$$

and the tunneling term is of the following form

$$H_T = \sum_{\mathbf{k}, \sigma, \alpha} (\tau_{\alpha} c_{\mathbf{k}\alpha, \sigma}^{\dagger} a_{\alpha, \sigma} + H.c.), \quad (4)$$

where α is the lead index (in $c_{\mathbf{k}\alpha, \sigma}^{\dagger}$), but also stands for the site where the lead is attached (in $a_{\alpha, \sigma}$); τ_{α} is the coupling constant. H_{int} may describe any interaction which implies the site "d", such as Hubbard or electron-phonon (photon) interaction, the electrostatic coupling to external detectors, etc. The equations of motion for the lesser Green functions can be written as [15]:

$$\sum_{k(\neq d)} (\delta_{ik} - g_i^r t_{ik}) G_{kj}^< = \tau_{\alpha}^2 g_{\alpha}^< g_i^r G_{ij}^a + g_i^r t_{id} G_{dj}^<, \quad i, j \neq d. \quad (5)$$

In the above equation we use the following notations: $g_i^r = (\omega - E_i + i\Gamma_i)^{-1}$ and $g_\alpha^< = 2i\pi\rho f_\alpha$ is the lesser Green function of the lead α which is coupled to the site "i"; ρ is the flat band density of states. The solution of eq.(5) reads

$$G_{ij}^< = (A^{-1})_{ik} (\tau_\alpha^2 g_\alpha^< g_k^r G_{kj}^a + g_k^r t_{kd} G_{dj}^<), \quad (6)$$

where the summation over "k" is assumed, and the notation $A_{ik} = \delta_{ik} - g_i^r t_{ik}$ have been used. The function $G_{dj}^<$ in eq.(6) can be obtained in a similar way:

$$G_{dj}^< = ((A^*)^{-1})_{jk} (\tau_\alpha^2 g_\alpha^< g_k^a G_{dk}^r + g_k^a t_{dk} G_{dd}^<) \quad (7)$$

where $g_k^a = (g_k^r)^*$.

One notices that $G_{ij}^<$ can be expressed in terms of the retarded (advanced) Green functions and $G_{dd}^<$. The calculation of $G_{dd}^<$ still remains a problem and several approximate solutions can be used, as for instance the Ng's ansatz described later. However, an important simplification occurs in the symmetric two-lead case when, after the symmetrization $J = (J_\alpha - J_\beta)/2$, the current becomes independent of $G_{dd}^<$:

$$J = \frac{2e}{h} \int d\omega \Gamma_\alpha (f_\alpha - f_\beta) \left\{ -\text{Im} G_{\alpha\alpha}^r + \sum_{\gamma(\neq d)} (A^{-1})_{\alpha\gamma} g_\gamma^r \left[(-1)^{\delta_{\alpha\gamma}} \Gamma_\gamma G_{\gamma\alpha}^a + t_{\gamma d} \sum_{\gamma'(\neq d)} (-1)^{\delta_{\alpha\gamma'}} ((A^*)^{-1})_{\alpha\gamma'} \Gamma_{\gamma'} g_{\gamma'}^a G_{d\gamma'}^r \right] \right\}. \quad (8)$$

The above equation represents the main formal result of this paper. The current J was expressed solely in terms of different retarded Green functions, for the symmetric case. The symmetry is necessary in order to get the same coefficient of $G_{dd}^<$ both in the expression of J_α and J_β , so that $G_{dd}^<$ is eliminated by the symmetrization $(J_\alpha - J_\beta)/2$. One can notice that the SIAM formula is recovered by the first term in eq.(8). Eq.(8) contains many retarded Green functions, but, in fact, all of them can be expressed in terms of G_{dd}^r , as for instance: $G_{d\gamma}^r = (A^{-1})_{\gamma\beta} g_\beta^r t_{d\beta} G_{dd}^r$.

Ng's ansatz . The lesser Green function $G^< = G^r \Sigma^< G^a$ is approximated by assuming that $\Sigma^< = \Sigma^{0<} M$ [14] where the matrix M is deduced from the relation $\Sigma^< - \Sigma^> = \Sigma^r - \Sigma^a$. The result is :

$$\Sigma^< = \Sigma^{0<} (\Sigma^{0r} - \Sigma^{0a})^{-1} (\Sigma^r - \Sigma^a). \quad (9)$$

The intention is again to keep in the final formula only retarded quantities and non-interacting functions (trivial to calculate). The non-interacting selfenergies , for the two lead system read :

$$\begin{aligned}\Sigma^{0<} &= \begin{pmatrix} f_\alpha & 0 \\ 0 & f_\beta \end{pmatrix} (\Sigma^{0r} - \Sigma^{0a}) \\ \Sigma^{0r} - \Sigma^{0a} &= -i \begin{pmatrix} \Gamma_\alpha & 0 \\ 0 & \Gamma_\beta \end{pmatrix}.\end{aligned}\tag{10}$$

It is now straightforward to express the quantities required by the current formula eq.(1) as :

$$\begin{aligned}G_{\alpha\alpha}^< &= -G_{\alpha\alpha}^r f_\alpha [(\Sigma^r - \Sigma^a)G^a]_{\alpha\alpha} - G_{\alpha\beta}^r f_\beta [(\Sigma^r - \Sigma^a)G^a]_{\beta\alpha} \\ f_\alpha (G^r - G^a)_{\alpha\alpha} &= f_\alpha [G^r(\Sigma^r - \Sigma^a)G^a]_{\alpha\alpha} = G_{\alpha\alpha}^r f_\alpha [(\Sigma^r - \Sigma^a)G^a]_{\alpha\alpha} + G_{\alpha\beta}^r f_\alpha [(\Sigma^r - \Sigma^a)G^a]_{\beta\alpha}.\end{aligned}\tag{11}$$

Finally, the current formula becomes :

$$J_\alpha = \frac{2ie}{h} \int d\omega (f_\alpha - f_\beta) \Gamma_\alpha G_{\alpha\beta}^r [(\Sigma^r - \Sigma^a)G^a]_{\beta\alpha}.\tag{12}$$

The same scheme was used in [16, 17], but for a different problem, namely the spin transport through a single-site dot coupled to magnetic leads.

III. APPLICATION AND DISCUSSIONS.

The exact formula eq.(8) will be applied to the particular case of a triangular interferometer with Hubbard interaction $H_{int} = U a_{d\uparrow}^\dagger a_{d\uparrow} a_{d\downarrow}^\dagger a_{d\downarrow}$. In the previous section, we reached our goal of expressing the current through the retarded Green functions only. One important advantage is that there are already recipes for computing these functions in different approximations. We shall use the scheme proposed by Entin-Wohlman *et al* [8] for $U \rightarrow \infty$. The choice is justified by the simple analytical formulae which have an easy implementation.

The triangular system is a good tool for studying the interplay between correlation and interference processes. The non-interacting conductance (curve no.3 in Fig.1) shows a typical Fano line presenting both a Fano zero and a perfect constructive interference. This is the result of the interference between the partial waves passing the dot and the reference arm.

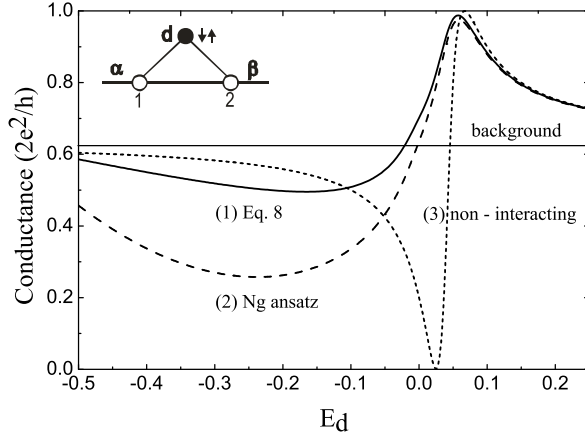


FIG. 1: Conductance through the triangular interferometer (see inset): (1) using exact formula (Eq.8), (2) with Ng's ansatz (Eq.12), and (3) for non-interacting case. The parameters are $E_1 = E_2 = E_{Fermi} = 0, \Gamma = 0.025, t_{12} = t_{1d} = t_{2d} = 0.02, T = 10^{-20}$ (measured in units of half-band width). The horizontal line represents the asymptotic value for E_d going to $\pm\infty$.

In the Kondo regime the dot transmits through the Kondo peak and the transmission phase is "frozen" at $\pi/2$ (as measured also experimentally in [18, 19]). The result consists in a much slower variation of the interference conditions giving rise to a Fano line of reduced amplitude compared to the non-interacting case. This is known as the Fano-Kondo effect and is described by the curve no.1 in Fig.1.

Significant differences can be noticed between the conductance obtained by using the exact formula eq.(8) and the Ng's approximation eq.(12) [20]. The differences are rather large, indicating that the Ng's ansatz does not capture well the combined effect of correlation and interference. Fig.1 shows that the destructive interference is overestimated. When the dot is empty ($E_d \gtrsim 0.1$) all the three curves coincide, as expected. The main control parameter (also in experiments) is the position on the energy scale of the atomic energy E_d which can be changed by applying an external bias. Asymptotically, for $|E_d| \rightarrow \infty$, the interacting site "d" is decoupled from the other sites; consequently the transport is performed only through the background branch (i.e., that one connecting the sites "1" and "2"). The background conductance is also plotted in Fig.1 and represents the control limit of our calculations. In the range of the gate potential where the correlations are important, the temperature dependence is expected to be of Kondo- type ,i.e. the conductance increases

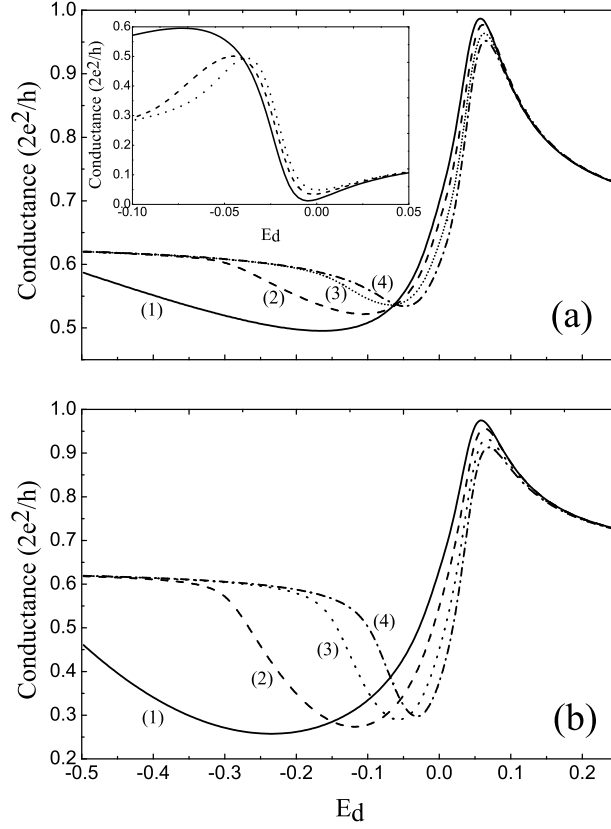


FIG. 2: a) The crossing point exhibited by the current curves calculated at different temperatures in the range $[T = 10^{-20} - 10^{-3}]$. Curve (1) is for the lowest temperature. Other parameters are the same as in Fig.1. The inset shows the same behavior for the T-shape system. b) The same curves calculated with Ng's approximation, which misses the crossing point.

with decreasing temperature. However, when multiple paths are possible (and interference plays an important role), an increased transparency of the quantum dot may give rise, on the contrary, to a reduced conductance of the whole system. The interference conditions can be changed by a magnetic field (as in [6]) or by variation of the gate potential as we are doing here.

The isotherms of the conductance $g = dJ/d\mu$ plotted in Fig.2 show two different temperature regimes separated by a crossing point: on the right the conductance decreases with T , and behaves oppositely on the left side. Our calculation determines the crossing point with an accuracy within numerical errors, and suggests that there is a gate potential E_d^c such that

$$dg(E_d^c, T)/dT = 0. \quad (13)$$

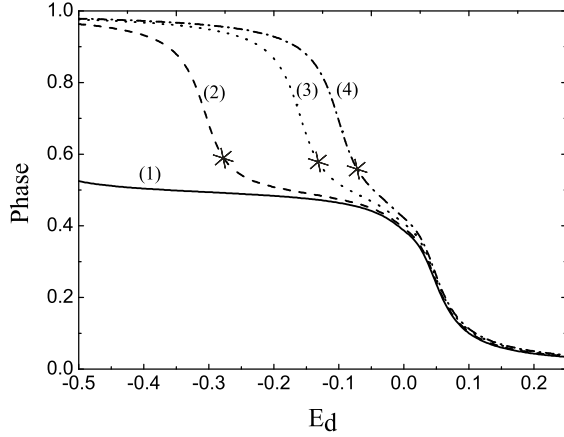


FIG. 3: The phase of G_{dd}^r (in units π) for the same parameters as in Fig.2; the stars indicate the gate potentials where the Kondo temperature equals the plot temperature. The curve (1) is still in Kondo regime at $E_d = -0.5$.

The same crossing point was found for a more simple model, namely the T-shape system. The T-shape geometry consists of two coupled quantum dots, only one of them (the non-interacting dot) being connected to leads. The advantage of this more simple model is that the conductance is simply expressed by the density of states at the site connected to leads (details are found in, e.g. [8]) and the effect of the interference is more obvious. Basically, the T-shape and the triangle describe the same Fano-Kondo physics; the triangle is however a technical challenge and the first step versus more realistic models.

The DoS at the Kondo dot always shows the specific Kondo peak at the Fermi energy. However, the DoS at the coupling site may show a Kondo peak or dip depending on the constructive or destructive interference conditions, respectively. The two cases give opposite temperature behavior. The interference conditions gradually change with the applied gate, giving rise to regions with opposite temperature dependence separated by a crossing point (see inset of Fig.2). The existence of this point seems to be a fingerprint of the Fano-Kondo effect in systems with interaction and interference. The use of the exact formula eq.8 is essential, since the Ng's approximation eq.12 misses the crossing point (as can be noticed in Fig.2b). This shows that the Ng's approximations fails not only quantitatively but also qualitatively.

If we intend to identify the gate interval where Kondo correlations are important, one

has to calculate the Kondo temperature. Another visualization of the Kondo region is to plot the phase of the dot Green function

$$\phi = \text{atan}(ImG_{dd}/ReG_{dd}), \quad (14)$$

that is known to "freeze" at the value $\pi/2$ in the Kondo regime. The phase is plotted in Fig.3 for several temperatures, and on each curve, we mark the point where the Kondo temperature equals the temperature of the curve. The Kondo temperature was computed with the Haldane [8, 21] formula. One can notice from Fig.3 that the crossing point $E_d \approx -0.05$ (see Fig.2) is indeed in the Kondo regime. For higher temperatures we have checked that the isotherms no longer pass through the crossing point as the transport is no more governed by the Kondo physics.

In conclusion, we have developed an exact current formula easy to apply to multiple-connected meso-systems. The advantage of the formula is that it uses only retarded Green functions and can be applied to any system with left-right and time reversal symmetry with one-site interaction. In the absence of the symmetries we give an alternative approach based on the Ng's ansatz, which nevertheless is not sufficiently accurate for describing the correlations. It has been found that the interplay between the Kondo correlation and the interference effect gives rise to different temperature behaviors depending on the gate potential applied on the interacting dot, separated by a crossing point.

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